



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 06:49 PM EDT

PDB ID : 7CK8  
Title : Crystal structure of human ferritin heavy chain mutant C90S/C102S/C130S  
Authors : Chen, X.; Jiang, B.; Yan, X.; Fan, K.  
Deposited on : 2020-07-16  
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

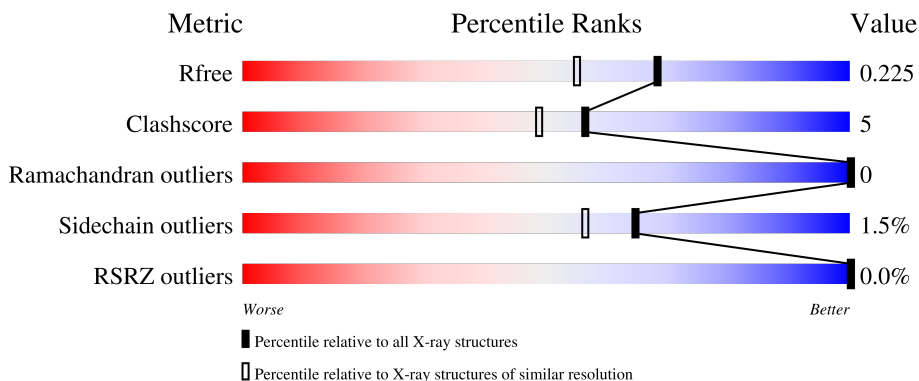
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	173	
1	B	173	
1	C	173	
1	D	173	
1	E	173	

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Mol	Chain	Length	Quality of chain
1	F	173	 87% 12% ..
1	G	173	 90% 10% .
1	H	173	 92% 8% .
1	I	173	 88% 11% .
1	J	173	 87% 12% .
1	K	173	 89% 10% .
1	L	173	 91% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	206	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 22459 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	Total 1580	C 997	N 277	O 302	S 4	0	23	0
1	B	172	Total 1568	C 985	N 276	O 303	S 4	0	20	0
1	C	172	Total 1609	C 1006	N 286	O 313	S 4	0	23	0
1	D	172	Total 1617	C 1020	N 283	O 310	S 4	0	27	0
1	E	172	Total 1555	C 982	N 272	O 297	S 4	0	20	0
1	F	172	Total 1567	C 982	N 279	O 302	S 4	0	19	0
1	G	173	Total 1588	C 999	N 281	O 304	S 4	0	23	0
1	H	173	Total 1588	C 1000	N 279	O 305	S 4	0	23	0
1	I	172	Total 1559	C 987	N 272	O 296	S 4	0	23	0
1	J	172	Total 1553	C 980	N 270	O 299	S 4	0	21	0
1	K	173	Total 1584	C 997	N 278	O 305	S 4	0	23	0
1	L	173	Total 1557	C 982	N 272	O 299	S 4	0	20	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	SER	CYS	engineered mutation	UNP P02794
A	102	SER	CYS	engineered mutation	UNP P02794
A	130	SER	CYS	engineered mutation	UNP P02794
B	90	SER	CYS	engineered mutation	UNP P02794
B	102	SER	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	130	SER	CYS	engineered mutation	UNP P02794
C	90	SER	CYS	engineered mutation	UNP P02794
C	102	SER	CYS	engineered mutation	UNP P02794
C	130	SER	CYS	engineered mutation	UNP P02794
D	90	SER	CYS	engineered mutation	UNP P02794
D	102	SER	CYS	engineered mutation	UNP P02794
D	130	SER	CYS	engineered mutation	UNP P02794
E	90	SER	CYS	engineered mutation	UNP P02794
E	102	SER	CYS	engineered mutation	UNP P02794
E	130	SER	CYS	engineered mutation	UNP P02794
F	90	SER	CYS	engineered mutation	UNP P02794
F	102	SER	CYS	engineered mutation	UNP P02794
F	130	SER	CYS	engineered mutation	UNP P02794
G	90	SER	CYS	engineered mutation	UNP P02794
G	102	SER	CYS	engineered mutation	UNP P02794
G	130	SER	CYS	engineered mutation	UNP P02794
H	90	SER	CYS	engineered mutation	UNP P02794
H	102	SER	CYS	engineered mutation	UNP P02794
H	130	SER	CYS	engineered mutation	UNP P02794
I	90	SER	CYS	engineered mutation	UNP P02794
I	102	SER	CYS	engineered mutation	UNP P02794
I	130	SER	CYS	engineered mutation	UNP P02794
J	90	SER	CYS	engineered mutation	UNP P02794
J	102	SER	CYS	engineered mutation	UNP P02794
J	130	SER	CYS	engineered mutation	UNP P02794
K	90	SER	CYS	engineered mutation	UNP P02794
K	102	SER	CYS	engineered mutation	UNP P02794
K	130	SER	CYS	engineered mutation	UNP P02794
L	90	SER	CYS	engineered mutation	UNP P02794
L	102	SER	CYS	engineered mutation	UNP P02794
L	130	SER	CYS	engineered mutation	UNP P02794

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	B	4	Total Cl 4 4	0	0
2	C	3	Total Cl 3 3	0	0
2	D	6	Total Cl 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	3	Total 3	Cl 3	0	0
2	F	5	Total 5	Cl 5	0	0
2	G	4	Total 4	Cl 4	0	0
2	H	3	Total 3	Cl 3	0	0
2	I	6	Total 6	Cl 6	0	0
2	J	3	Total 3	Cl 3	0	0
2	K	3	Total 3	Cl 3	0	0
2	L	2	Total 2	Cl 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Mg 3	0	0
3	B	2	Total 2	Mg 2	0	0
3	C	2	Total 2	Mg 2	0	0
3	D	2	Total 2	Mg 2	0	0
3	E	2	Total 2	Mg 2	0	0
3	F	2	Total 2	Mg 2	0	0
3	G	3	Total 3	Mg 3	0	0
3	H	4	Total 4	Mg 4	0	0
3	I	3	Total 3	Mg 3	0	0
3	J	2	Total 2	Mg 2	0	0
3	K	2	Total 2	Mg 2	0	0

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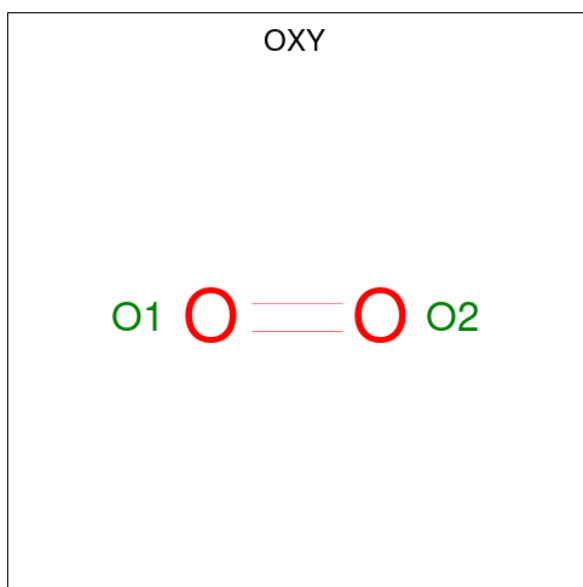
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	2	Total	Mg	0	0
			2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula:  $O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	C	1	Total O 2 2	0	0
5	C	1	Total O 2 2	0	0
5	C	1	Total O 2 2	0	0
5	D	1	Total O 2 2	0	0
5	E	1	Total O 2 2	0	0
5	E	1	Total O 2 2	0	0
5	F	1	Total O 2 2	0	0
5	G	1	Total O 2 2	0	0
5	G	1	Total O 2 2	0	0
5	H	1	Total O 2 2	0	0
5	I	1	Total O 2 2	0	0
5	I	1	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total O 2 2	0	0

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Fe 1 1	0	0

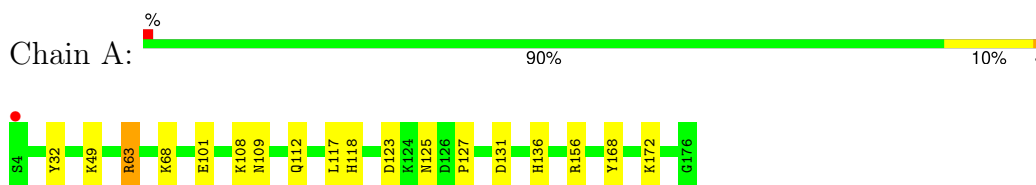
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	287	Total O 287 287	0	0
7	B	288	Total O 288 288	0	0
7	C	286	Total O 286 286	0	0
7	D	285	Total O 285 285	0	0
7	E	274	Total O 274 274	0	0
7	F	280	Total O 280 280	0	0
7	G	280	Total O 280 280	0	0
7	H	283	Total O 283 283	0	0
7	I	284	Total O 284 284	0	0
7	J	281	Total O 281 281	0	0
7	K	282	Total O 282 282	0	0
7	L	283	Total O 283 283	0	0

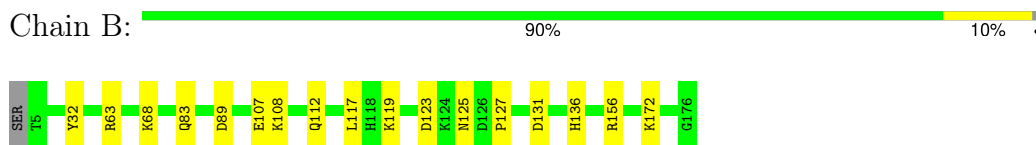
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

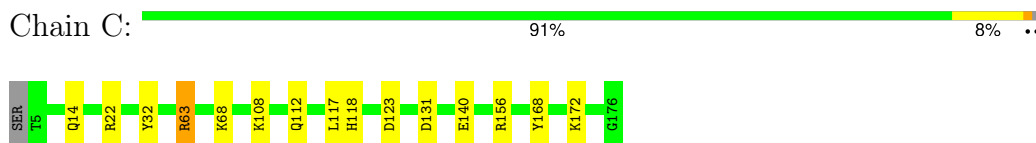
- Molecule 1: Ferritin heavy chain



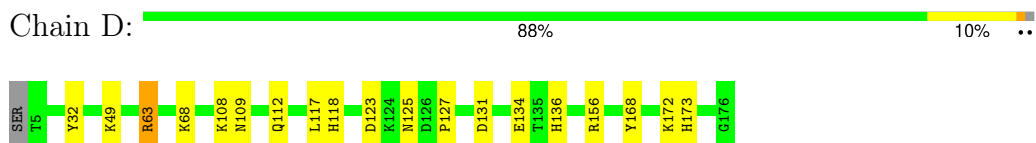
- Molecule 1: Ferritin heavy chain



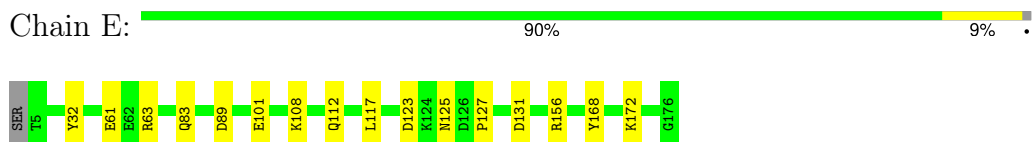
- Molecule 1: Ferritin heavy chain



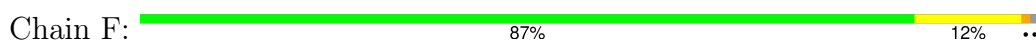
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

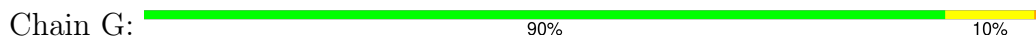


- Molecule 1: Ferritin heavy chain





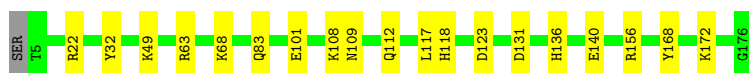
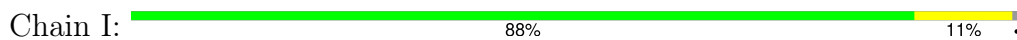
- Molecule 1: Ferritin heavy chain



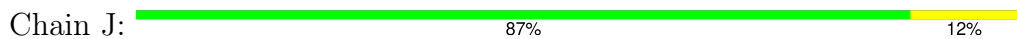
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.91Å 183.27Å 183.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.98 – 1.80 29.72 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.98-1.80) 99.5 (29.72-1.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 1.70Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.192 , 0.223 0.194 , 0.225	Depositor DCC
$R_{free}$ test set	16248 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.450 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	22459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8063e-11. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, GOL, MG, OXY, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.60	0/1654	0.68	2/2215 (0.1%)
1	B	0.59	0/1621	0.68	2/2171 (0.1%)
1	C	0.59	0/1656	0.67	2/2218 (0.1%)
1	D	0.58	0/1691	0.67	2/2264 (0.1%)
1	E	0.58	0/1620	0.67	2/2170 (0.1%)
1	F	0.60	0/1614	0.69	2/2162 (0.1%)
1	G	0.60	0/1653	0.67	2/2214 (0.1%)
1	H	0.59	0/1653	0.67	2/2215 (0.1%)
1	I	0.59	0/1648	0.67	2/2207 (0.1%)
1	J	0.60	0/1627	0.69	2/2181 (0.1%)
1	K	0.60	0/1652	0.69	2/2214 (0.1%)
1	L	0.59	0/1625	0.68	2/2178 (0.1%)
All	All	0.59	0/19714	0.68	24/26409 (0.1%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	63[A]	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	K	63[B]	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	63[A]	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	63[B]	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	F	63[A]	ARG	NE-CZ-NH2	-8.82	115.89	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1580	0	1579	16	0
1	B	1568	0	1539	14	0
1	C	1609	0	1567	17	0
1	D	1617	0	1612	18	0
1	E	1555	0	1548	15	0
1	F	1567	0	1532	19	0
1	G	1588	0	1576	18	0
1	H	1588	0	1573	13	0
1	I	1559	0	1573	18	0
1	J	1553	0	1544	14	0
1	K	1584	0	1571	17	0
1	L	1557	0	1547	12	0
2	A	3	0	0	0	0
2	B	4	0	0	1	0
2	C	3	0	0	1	0
2	D	6	0	0	1	0
2	E	3	0	0	1	0
2	F	5	0	0	0	0
2	G	4	0	0	1	0
2	H	3	0	0	1	0
2	I	6	0	0	2	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	2	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	4	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	1	0
4	C	6	0	8	4	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	I	6	0	8	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	6	0	0	1	0
5	D	2	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
5	G	4	0	0	0	0
5	H	2	0	0	0	0
5	I	4	0	0	0	0
5	L	2	0	0	0	0
6	D	1	0	0	0	0
7	A	287	0	0	10	2
7	B	288	0	0	10	5
7	C	286	0	0	15	2
7	D	285	0	0	12	2
7	E	274	0	0	10	5
7	F	280	0	0	13	6
7	G	280	0	0	13	4
7	H	283	0	0	9	13
7	I	284	0	0	14	0
7	J	281	0	0	12	4
7	K	282	0	0	12	4
7	L	283	0	0	9	13
All	All	22459	0	18809	189	30

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 189 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156[A]:ARG:NH1	7:F:301:HOH:O	1.91	1.01
1:J:156[A]:ARG:NH1	7:J:301:HOH:O	1.94	1.00
1:K:156[A]:ARG:NH1	7:K:301:HOH:O	1.95	0.99
1:D:156[B]:ARG:NH1	7:D:301:HOH:O	1.95	0.99
1:I:156[A]:ARG:NH1	7:I:301:HOH:O	1.95	0.98

The worst 5 of 30 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:577:HOH:O	7:E:547:HOH:O[8_455]	2.01	0.19
7:E:547:HOH:O	7:G:351:HOH:O[8_555]	2.02	0.18
7:B:558:HOH:O	7:E:568:HOH:O[8_455]	2.03	0.17
7:B:558:HOH:O	7:K:342:HOH:O[8_455]	2.04	0.16
7:H:319:HOH:O	7:K:313:HOH:O[3_555]	2.05	0.15

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	194/173 (112%)	190 (98%)	4 (2%)	0	100	100
1	B	190/173 (110%)	187 (98%)	3 (2%)	0	100	100
1	C	193/173 (112%)	190 (98%)	3 (2%)	0	100	100
1	D	198/173 (114%)	194 (98%)	4 (2%)	0	100	100
1	E	190/173 (110%)	187 (98%)	3 (2%)	0	100	100
1	F	189/173 (109%)	187 (99%)	2 (1%)	0	100	100
1	G	194/173 (112%)	190 (98%)	4 (2%)	0	100	100
1	H	194/173 (112%)	191 (98%)	3 (2%)	0	100	100
1	I	193/173 (112%)	190 (98%)	3 (2%)	0	100	100
1	J	190/173 (110%)	186 (98%)	4 (2%)	0	100	100
1	K	194/173 (112%)	190 (98%)	4 (2%)	0	100	100
1	L	191/173 (110%)	188 (98%)	3 (2%)	0	100	100
All	All	2310/2076 (111%)	2270 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/154 (115%)	174 (98%)	3 (2%)	60	51
1	B	173/154 (112%)	170 (98%)	3 (2%)	60	51
1	C	177/154 (115%)	174 (98%)	3 (2%)	60	51
1	D	181/154 (118%)	178 (98%)	3 (2%)	60	51
1	E	173/154 (112%)	170 (98%)	3 (2%)	60	51
1	F	172/154 (112%)	169 (98%)	3 (2%)	60	51
1	G	177/154 (115%)	174 (98%)	3 (2%)	60	51
1	H	177/154 (115%)	174 (98%)	3 (2%)	60	51
1	I	176/154 (114%)	173 (98%)	3 (2%)	60	51
1	J	174/154 (113%)	169 (97%)	5 (3%)	42	29
1	K	177/154 (115%)	173 (98%)	4 (2%)	50	37
1	L	174/154 (113%)	169 (97%)	5 (3%)	42	29
All	All	2108/1848 (114%)	2067 (98%)	41 (2%)	65	46

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	49[A]	LYS
1	K	117[B]	LEU
1	J	49[B]	LYS
1	K	32	TYR
1	L	49[A]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	173	HIS
1	E	83	GLN
1	G	83	GLN
1	I	83	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 75 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	OXY	C	207	-	1,1,1	0.12	0	-		
5	OXY	G	208	-	1,1,1	0.10	0	-		
5	OXY	L	205	-	1,1,1	0.12	0	-		
5	OXY	E	207	-	1,1,1	0.17	0	-		
4	GOL	A	207	-	5,5,5	1.91	2 (40%)	5,5,5	1.47	1 (20%)
5	OXY	E	208	-	1,1,1	0.10	0	-		
5	OXY	B	208	-	1,1,1	0.20	0	-		
5	OXY	F	208	-	1,1,1	0.02	0	-		
4	GOL	B	207	-	5,5,5	1.65	1 (20%)	5,5,5	1.41	1 (20%)
5	OXY	I	212	-	1,1,1	0.08	0	-		
5	OXY	C	209	-	1,1,1	0.08	0	-		
5	OXY	A	208	-	1,1,1	0.01	0	-		
4	GOL	D	210	-	5,5,5	0.84	0	5,5,5	1.36	1 (20%)
5	OXY	C	208	-	1,1,1	0.07	0	-		
4	GOL	I	210	-	5,5,5	1.28	0	5,5,5	1.26	1 (20%)
5	OXY	H	208	-	1,1,1	0.02	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	C	206	-	5,5,5	1.08	1 (20%)	5,5,5	1.18	0
5	OXY	I	211	-	1,1,1	0.08	0	-		
5	OXY	G	209	-	1,1,1	0.11	0	-		
4	GOL	E	206	-	5,5,5	1.57	1 (20%)	5,5,5	1.44	1 (20%)
5	OXY	D	211	-	1,1,1	0.14	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	206	-	-	4/4/4/4	-
4	GOL	D	210	-	-	2/4/4/4	-
4	GOL	B	207	-	-	2/4/4/4	-
4	GOL	I	210	-	-	2/4/4/4	-
4	GOL	E	206	-	-	2/4/4/4	-
4	GOL	A	207	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	207	GOL	O2-C2	3.42	1.53	1.43
4	B	207	GOL	O2-C2	2.94	1.51	1.43
4	E	206	GOL	O2-C2	2.74	1.51	1.43
4	C	206	GOL	O2-C2	-2.21	1.37	1.43
4	A	207	GOL	C3-C2	2.21	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	207	GOL	C3-C2-C1	-3.02	100.72	111.80
4	E	206	GOL	C3-C2-C1	-2.85	101.33	111.80
4	B	207	GOL	C3-C2-C1	-2.78	101.58	111.80
4	D	210	GOL	C3-C2-C1	-2.61	102.22	111.80
4	I	210	GOL	C3-C2-C1	-2.42	102.93	111.80

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	207	GOL	C1-C2-C3-O3
4	A	207	GOL	O2-C2-C3-O3
4	B	207	GOL	C1-C2-C3-O3
4	C	206	GOL	C1-C2-C3-O3
4	D	210	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	207	OXY	1	0
4	B	207	GOL	1	0
4	C	206	GOL	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	173/173 (100%)	-0.93	1 (0%) 89   87	13, 16, 24, 68	0
1	B	172/173 (99%)	-1.01	0 100   100	13, 16, 24, 37	0
1	C	172/173 (99%)	-0.99	0 100   100	12, 16, 24, 37	0
1	D	172/173 (99%)	-0.94	0 100   100	13, 16, 24, 40	0
1	E	172/173 (99%)	-1.01	0 100   100	13, 16, 24, 38	0
1	F	172/173 (99%)	-1.01	0 100   100	12, 16, 24, 39	0
1	G	173/173 (100%)	-0.97	0 100   100	13, 16, 25, 66	0
1	H	173/173 (100%)	-0.98	0 100   100	12, 16, 24, 61	0
1	I	172/173 (99%)	-0.98	0 100   100	12, 16, 24, 37	0
1	J	172/173 (99%)	-1.00	0 100   100	13, 16, 24, 38	0
1	K	173/173 (100%)	-0.97	0 100   100	13, 16, 24, 65	1 (0%)
1	L	173/173 (100%)	-0.98	0 100   100	13, 16, 24, 62	0
All	All	2069/2076 (99%)	-0.98	1 (0%) 100   100	12, 16, 24, 68	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	SER	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	D	210	6/6	0.51	0.17	44,47,47,54	0
4	GOL	I	210	6/6	0.62	0.15	38,41,44,44	0
4	GOL	A	207	6/6	0.63	0.18	34,36,41,42	0
4	GOL	B	207	6/6	0.73	0.14	36,38,41,42	0
4	GOL	E	206	6/6	0.76	0.14	35,39,41,43	0
4	GOL	C	206	6/6	0.85	0.13	32,43,46,50	0
3	MG	H	206	1/1	0.85	0.31	56,56,56,56	0
5	OXY	A	208	2/2	0.88	0.10	28,28,28,38	0
5	OXY	C	207	2/2	0.88	0.14	44,44,44,56	0
5	OXY	H	208	2/2	0.89	0.11	32,32,32,42	0
2	CL	H	202	1/1	0.91	0.18	47,47,47,47	0
3	MG	F	207	1/1	0.91	0.07	33,33,33,33	0
3	MG	J	205	1/1	0.92	0.07	32,32,32,32	0
3	MG	C	205	1/1	0.93	0.08	33,33,33,33	0
3	MG	D	208	1/1	0.93	0.07	32,32,32,32	0
3	MG	A	205	1/1	0.93	0.06	33,33,33,33	0
3	MG	G	207	1/1	0.93	0.08	33,33,33,33	0
5	OXY	D	211	2/2	0.93	0.20	36,36,36,41	0
3	MG	A	206	1/1	0.93	0.08	36,36,36,36	0
3	MG	I	209	1/1	0.94	0.07	32,32,32,32	0
5	OXY	E	207	2/2	0.94	0.14	37,37,37,39	0
5	OXY	F	208	2/2	0.94	0.08	28,28,28,39	0
3	MG	K	205	1/1	0.94	0.07	33,33,33,33	0
3	MG	H	207	1/1	0.95	0.07	35,35,35,35	0
5	OXY	G	208	2/2	0.95	0.18	35,35,35,44	0
5	OXY	G	209	2/2	0.95	0.10	30,30,30,37	0
2	CL	D	202	1/1	0.95	0.13	46,46,46,46	0
5	OXY	I	212	2/2	0.95	0.11	30,30,30,37	0
6	FE	D	209	1/1	0.95	0.07	59,59,59,59	0
3	MG	L	204	1/1	0.96	0.07	33,33,33,33	0
3	MG	H	205	1/1	0.96	0.04	35,35,35,35	0
3	MG	G	206	1/1	0.96	0.04	35,35,35,35	0
5	OXY	E	208	2/2	0.96	0.17	31,31,31,43	0
2	CL	E	201	1/1	0.96	0.10	39,39,39,39	0
3	MG	B	206	1/1	0.97	0.09	31,31,31,31	0
5	OXY	B	208	2/2	0.97	0.14	37,37,37,40	0
3	MG	E	205	1/1	0.97	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	OXY	C	209	2/2	0.98	0.09	29,29,29,41	0
2	CL	F	202	1/1	0.98	0.14	49,49,49,49	0
2	CL	I	201	1/1	0.98	0.05	32,32,32,32	0
5	OXY	I	211	2/2	0.98	0.08	29,29,29,41	0
2	CL	F	203	1/1	0.98	0.20	47,47,47,47	0
5	OXY	L	205	2/2	0.98	0.12	28,28,28,37	0
5	OXY	C	208	2/2	0.98	0.15	33,33,33,43	0
3	MG	I	207	1/1	0.99	0.07	24,24,24,24	0
2	CL	C	201	1/1	0.99	0.04	22,22,22,22	0
2	CL	A	202	1/1	0.99	0.03	31,31,31,31	0
3	MG	K	204	1/1	0.99	0.07	15,15,15,15	0
2	CL	I	204	1/1	0.99	0.04	22,22,22,22	0
2	CL	I	205	1/1	0.99	0.15	39,39,39,39	0
2	CL	I	206	1/1	0.99	0.06	28,28,28,28	0
2	CL	J	201	1/1	0.99	0.04	22,22,22,22	0
2	CL	J	202	1/1	0.99	0.04	24,24,24,24	0
2	CL	J	203	1/1	0.99	0.03	30,30,30,30	0
2	CL	K	201	1/1	0.99	0.04	24,24,24,24	0
2	CL	K	202	1/1	0.99	0.03	31,31,31,31	0
2	CL	K	203	1/1	0.99	0.04	21,21,21,21	0
2	CL	L	201	1/1	0.99	0.04	21,21,21,21	0
3	MG	A	204	1/1	0.99	0.08	15,15,15,15	0
2	CL	D	203	1/1	0.99	0.03	31,31,31,31	0
2	CL	D	204	1/1	0.99	0.04	21,21,21,21	0
2	CL	D	205	1/1	0.99	0.05	28,28,28,28	0
2	CL	D	206	1/1	0.99	0.04	17,17,17,17	0
2	CL	A	203	1/1	0.99	0.04	21,21,21,21	0
2	CL	B	201	1/1	0.99	0.04	21,21,21,21	0
2	CL	B	202	1/1	0.99	0.04	27,27,27,27	0
3	MG	G	205	1/1	0.99	0.08	15,15,15,15	0
2	CL	F	204	1/1	0.99	0.04	24,24,24,24	0
2	CL	F	205	1/1	0.99	0.03	30,30,30,30	0
2	CL	G	201	1/1	0.99	0.04	24,24,24,24	0
2	CL	G	202	1/1	0.99	0.04	31,31,31,31	0
2	CL	G	204	1/1	0.99	0.06	29,29,29,29	0
3	MG	L	203	1/1	1.00	0.06	15,15,15,15	0
2	CL	I	203	1/1	1.00	0.04	16,16,16,16	1
3	MG	C	204	1/1	1.00	0.09	14,14,14,14	0
2	CL	B	203	1/1	1.00	0.05	24,24,24,24	0
3	MG	D	207	1/1	1.00	0.06	15,15,15,15	0
2	CL	B	204	1/1	1.00	0.03	16,16,16,16	0
3	MG	E	204	1/1	1.00	0.07	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	201	1/1	1.00	0.04	25,25,25,25	0
3	MG	F	206	1/1	1.00	0.08	14,14,14,14	0
2	CL	C	202	1/1	1.00	0.05	24,24,24,24	0
2	CL	C	203	1/1	1.00	0.04	16,16,16,16	1
2	CL	D	201	1/1	1.00	0.04	25,25,25,25	0
2	CL	G	203	1/1	1.00	0.04	21,21,21,21	0
3	MG	H	204	1/1	1.00	0.06	15,15,15,15	0
2	CL	E	202	1/1	1.00	0.04	21,21,21,21	0
2	CL	H	201	1/1	1.00	0.03	24,24,24,24	0
2	CL	E	203	1/1	1.00	0.03	27,27,27,27	0
2	CL	L	202	1/1	1.00	0.03	24,24,24,24	0
3	MG	I	208	1/1	1.00	0.09	14,14,14,14	0
2	CL	H	203	1/1	1.00	0.04	21,21,21,21	0
3	MG	J	204	1/1	1.00	0.07	14,14,14,14	0
2	CL	F	201	1/1	1.00	0.04	22,22,22,22	0
2	CL	I	202	1/1	1.00	0.05	24,24,24,24	0
3	MG	B	205	1/1	1.00	0.06	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.